Full wwPDB X-ray Structure Validation Report ⓘ

Oct 31, 2023 – 06:08 PM EDT

PDB ID	:	8TXN
Title	:	Adaptive mechanism of collagen IV scaffold assembly in Drosophila: crystal structure of recombinant NC1 hexamer
Authors	:	Boudko, S.P.
Deposited on	:	2023-08-23
Resolution	:	1.75 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

The following versions of software and data (see references ⓘ) were used in the production of this report:

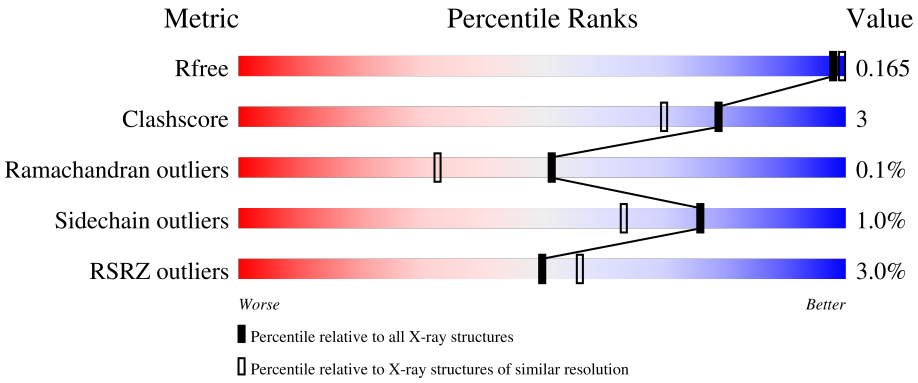
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 1.75 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	2340 (1.76-1.76)
Clashscore	141614	2466 (1.76-1.76)
Ramachandran outliers	138981	2437 (1.76-1.76)
Sidechain outliers	138945	2437 (1.76-1.76)
RSRZ outliers	127900	2298 (1.76-1.76)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	726	2% 86% 7% 7%
1	D	726	4% 87% 6% 7%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
6	PEG	A	3009	-	-	X	-

2 Entry composition (i)

There are 10 unique types of molecules in this entry. The entry contains 11574 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Collagen alpha-1(IV) chain, Collagen IV - chain Viking, Collagen alpha-1(IV) chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	674	Total	C	N	O	S	0	15	0
			5260	3281	917	1003	59			
1	D	676	Total	C	N	O	S	0	15	0
			5296	3311	920	1005	60			

There are 72 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-16	ALA	-	expression tag	UNP P08120
A	-15	PRO	-	expression tag	UNP P08120
A	-14	LEU	-	expression tag	UNP P08120
A	-13	ALA	-	expression tag	UNP P08120
A	-12	ASP	-	expression tag	UNP P08120
A	-11	TYR	-	expression tag	UNP P08120
A	-10	LYS	-	expression tag	UNP P08120
A	-9	ASP	-	expression tag	UNP P08120
A	-8	ASP	-	expression tag	UNP P08120
A	-7	ASP	-	expression tag	UNP P08120
A	-6	ASP	-	expression tag	UNP P08120
A	-5	LYS	-	expression tag	UNP P08120
A	-4	LEU	-	expression tag	UNP P08120
A	-3	ALA	-	expression tag	UNP P08120
A	-2	SER	-	expression tag	UNP P08120
A	-1	THR	-	expression tag	UNP P08120
A	230	GLY	-	linker	UNP P08120
A	231	SER	-	linker	UNP P08120
A	232	SER	-	linker	UNP P08120
A	233	ALA	-	linker	UNP P08120
A	234	SER	-	linker	UNP P08120
A	235	SER	-	linker	UNP P08120
A	236	GLY	-	linker	UNP P08120
A	1230	GLY	-	linker	UNP Q9VMV5

Continued on next page...

Continued from previous page...

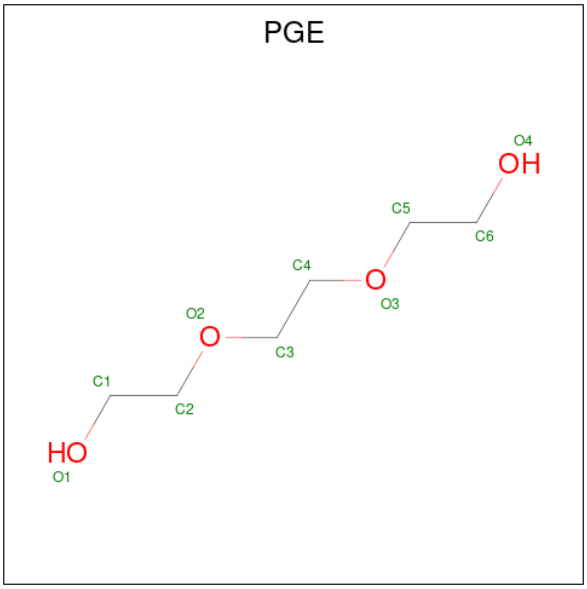
Chain	Residue	Modelled	Actual	Comment	Reference
A	1231	SER	-	linker	UNP Q9VMV5
A	1232	SER	-	linker	UNP Q9VMV5
A	1233	ALA	-	linker	UNP Q9VMV5
A	1234	SER	-	linker	UNP Q9VMV5
A	1235	SER	-	linker	UNP Q9VMV5
A	1236	GLY	-	linker	UNP Q9VMV5
A	2230	GLY	-	cloning artifact	UNP P08120
A	2231	SER	-	cloning artifact	UNP P08120
A	2232	GLY	-	cloning artifact	UNP P08120
A	2233	SER	-	cloning artifact	UNP P08120
A	2234	GLY	-	cloning artifact	UNP P08120
A	2235	SER	-	cloning artifact	UNP P08120
D	-16	ALA	-	expression tag	UNP P08120
D	-15	PRO	-	expression tag	UNP P08120
D	-14	LEU	-	expression tag	UNP P08120
D	-13	ALA	-	expression tag	UNP P08120
D	-12	ASP	-	expression tag	UNP P08120
D	-11	TYR	-	expression tag	UNP P08120
D	-10	LYS	-	expression tag	UNP P08120
D	-9	ASP	-	expression tag	UNP P08120
D	-8	ASP	-	expression tag	UNP P08120
D	-7	ASP	-	expression tag	UNP P08120
D	-6	ASP	-	expression tag	UNP P08120
D	-5	LYS	-	expression tag	UNP P08120
D	-4	LEU	-	expression tag	UNP P08120
D	-3	ALA	-	expression tag	UNP P08120
D	-2	SER	-	expression tag	UNP P08120
D	-1	THR	-	expression tag	UNP P08120
D	230	GLY	-	linker	UNP P08120
D	231	SER	-	linker	UNP P08120
D	232	SER	-	linker	UNP P08120
D	233	ALA	-	linker	UNP P08120
D	234	SER	-	linker	UNP P08120
D	235	SER	-	linker	UNP P08120
D	236	GLY	-	linker	UNP P08120
D	1230	GLY	-	linker	UNP Q9VMV5
D	1231	SER	-	linker	UNP Q9VMV5
D	1232	SER	-	linker	UNP Q9VMV5
D	1233	ALA	-	linker	UNP Q9VMV5
D	1234	SER	-	linker	UNP Q9VMV5
D	1235	SER	-	linker	UNP Q9VMV5
D	1236	GLY	-	linker	UNP Q9VMV5

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
D	2230	GLY	-	cloning artifact	UNP P08120
D	2231	SER	-	cloning artifact	UNP P08120
D	2232	GLY	-	cloning artifact	UNP P08120
D	2233	SER	-	cloning artifact	UNP P08120
D	2234	GLY	-	cloning artifact	UNP P08120
D	2235	SER	-	cloning artifact	UNP P08120

- Molecule 2 is TRIETHYLENE GLYCOL (three-letter code: PGE) (formula: $C_6H_{14}O_4$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total C O 10 6 4	0	0
2	A	1	Total C O 10 6 4	0	0
2	A	1	Total C O 10 6 4	0	0
2	D	1	Total C O 10 6 4	0	0
2	D	1	Total C O 10 6 4	0	0

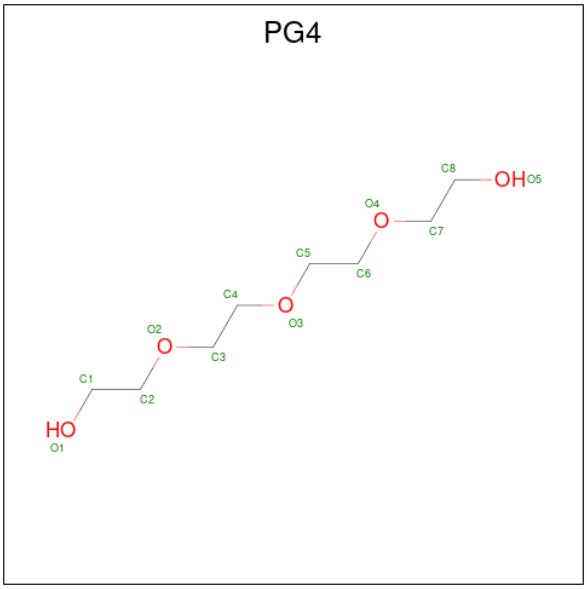
- Molecule 3 is CHLORIDE ION (three-letter code: CL) (formula: Cl) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	2	Total Cl 2 2	0	0
3	D	2	Total Cl 2 2	0	0

- Molecule 4 is MAGNESIUM ION (three-letter code: MG) (formula: Mg) (labeled as "Ligand of Interest" by depositor).

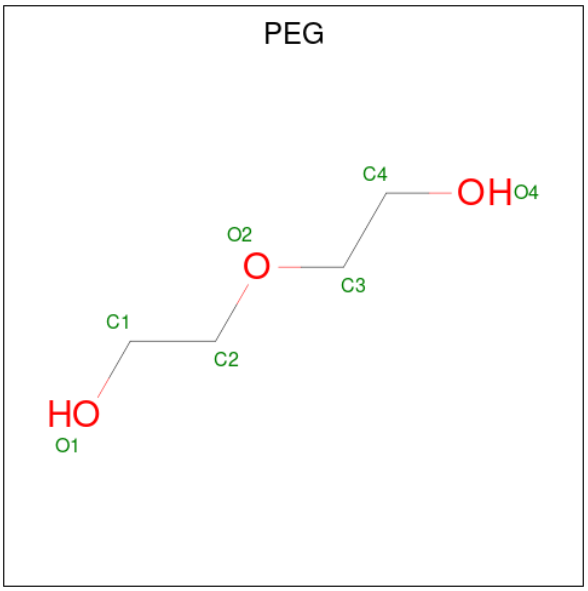
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total Mg 1 1	0	0
4	D	1	Total Mg 1 1	0	0

- Molecule 5 is TETRAETHYLENE GLYCOL (three-letter code: PG4) (formula: $C_8H_{18}O_5$).



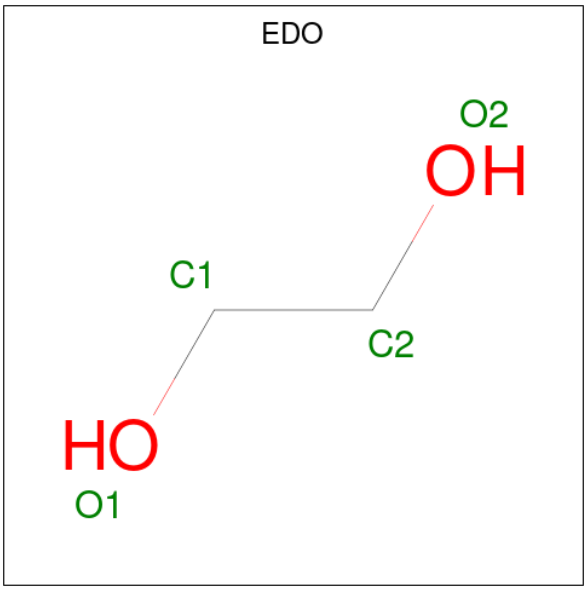
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	1	Total C O 13 8 5	0	0
5	D	1	Total C O 13 8 5	0	0

- Molecule 6 is DI(HYDROXYETHYL)ETHER (three-letter code: PEG) (formula: $C_4H_{10}O_3$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	1	Total C O 7 4 3	0	0
6	A	1	Total C O 7 4 3	0	0
6	D	1	Total C O 7 4 3	0	0

- Molecule 7 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: $C_2H_6O_2$).



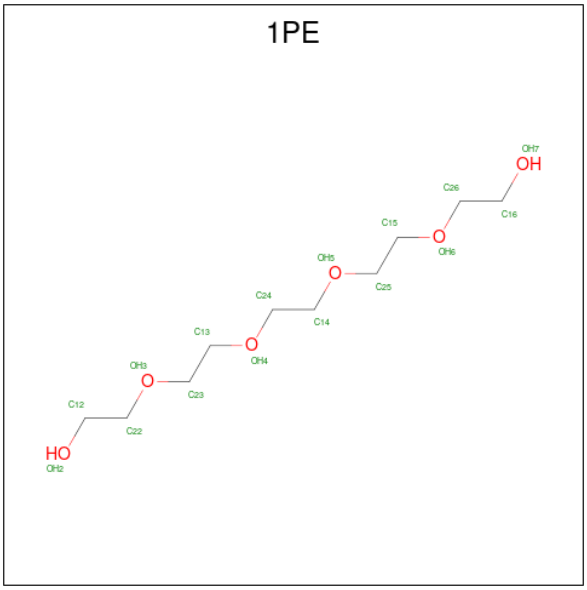
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	A	1	Total C O 4 2 2	0	0

Continued on next page...

Continued from previous page...

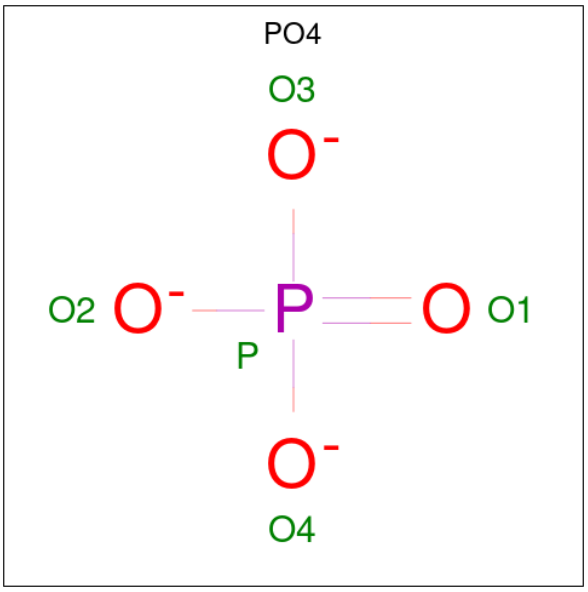
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	D	1	Total C O 4 2 2	0	0
7	D	1	Total C O 4 2 2	0	0
7	D	1	Total C O 4 2 2	0	0

- Molecule 8 is PENTAETHYLENE GLYCOL (three-letter code: 1PE) (formula: $C_{10}H_{22}O_6$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	D	1	Total C O 16 10 6	0	0
8	D	1	Total C O 16 10 6	0	0

- Molecule 9 is PHOSPHATE ION (three-letter code: PO4) (formula: O_4P).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
9	D	1	Total O P 5 4 1	0	0

- Molecule 10 is water.

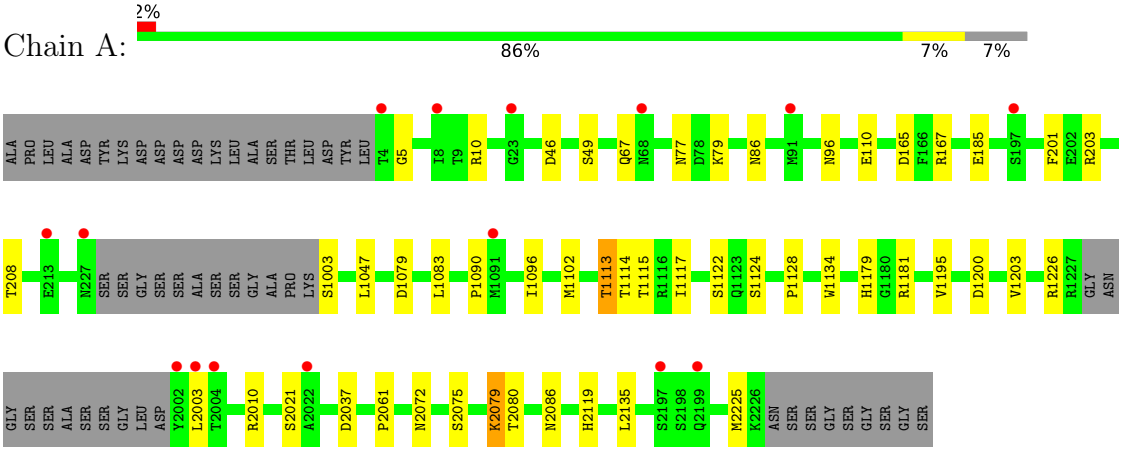
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
10	A	433	Total O 433 433	0	0
10	D	429	Total O 429 429	0	0

3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density (RSRZ > 2). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

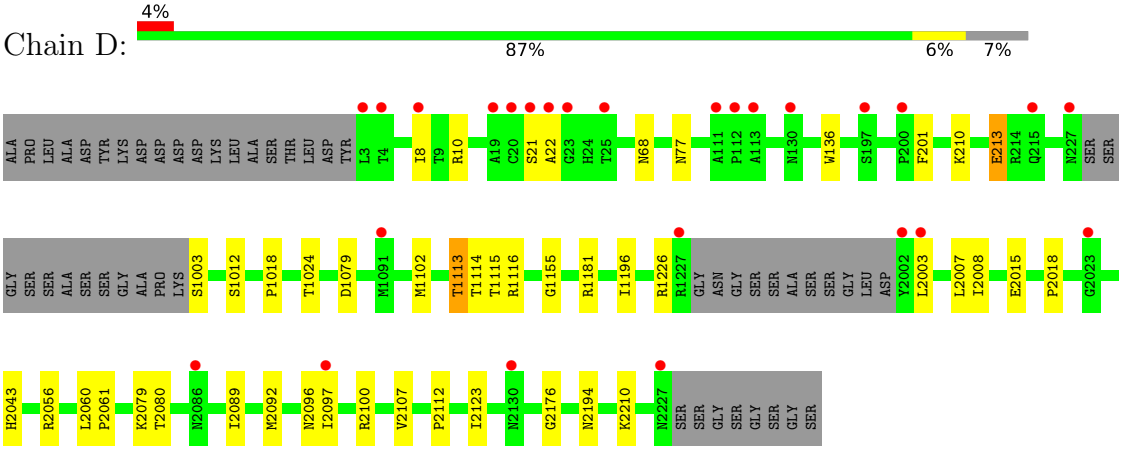
• Molecule 1: Collagen alpha-1(IV) chain, Collagen IV - chain Viking, Collagen alpha-1(IV) chain

Chain A:



• Molecule 1: Collagen alpha-1(IV) chain, Collagen IV - chain Viking, Collagen alpha-1(IV) chain

Chain D:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 63	Depositor
Cell constants a, b, c, α, β, γ	139.12Å 139.12Å 103.38Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	51.69 – 1.75 52.05 – 1.75	Depositor EDS
% Data completeness (in resolution range)	100.0 (51.69-1.75) 98.5 (52.05-1.75)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	4.09 (at 1.75Å)	Xtriage
Refinement program	PHENIX 1.20.1_4487	Depositor
R, R_{free}	0.142 , 0.164 0.142 , 0.165	Depositor DCC
R_{free} test set	2003 reflections (1.75%)	wwPDB-VP
Wilson B-factor (Å^2)	16.5	Xtriage
Anisotropy	0.310	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.38 , 52.8	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	0.031 for h,-h-k,-l	Xtriage
F_o,F_c correlation	0.97	EDS
Total number of atoms	11574	wwPDB-VP
Average B, all atoms (Å^2)	23.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.72% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: EDO, CL, 1PE, PO4, PG4, MG, PGE, PEG

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\| > 5$	RMSZ	$\#\|Z\| > 5$
1	A	0.35	0/5436	0.60	0/7397
1	D	0.35	0/5476	0.61	0/7451
All	All	0.35	0/10912	0.61	0/14848

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	5260	0	4987	30	0
1	D	5296	0	5049	27	0
2	A	30	0	42	2	0
2	D	20	0	28	1	0
3	A	2	0	0	0	0
3	D	2	0	0	0	0
4	A	1	0	0	0	0
4	D	1	0	0	0	0
5	A	13	0	18	0	0
5	D	13	0	18	0	0
6	A	14	0	20	4	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	D	7	0	10	0	0
7	A	4	0	6	0	0
7	D	12	0	18	1	0
8	D	32	0	44	2	0
9	D	5	0	0	0	0
10	A	433	0	0	3	0
10	D	429	0	0	2	0
All	All	11574	0	10240	58	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 3.

All (58) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2119:HIS:H	6:A:3009:PEG:H32	1.43	0.84
1:A:77[B]:ASN:ND2	10:A:4001:HOH:O	2.21	0.74
1:D:10:ARG:NH2	1:D:21:SER:OG	2.21	0.73
1:D:2015:GLU:OE1	1:D:2100[B]:ARG:NH1	2.23	0.70
1:A:2119:HIS:N	6:A:3009:PEG:H32	2.06	0.68
1:A:2135:LEU:HD21	1:A:2225:MET:HE2	1.75	0.68
1:A:2061:PRO:HD2	1:A:2080:THR:HG21	1.81	0.63
1:A:201:PHE:CE2	1:A:1102:MET:HG2	2.39	0.58
1:A:1115:THR:HB	1:A:1226:ARG:HB3	1.87	0.56
1:A:201:PHE:CZ	1:A:1102:MET:HG2	2.40	0.56
1:D:1115:THR:HB	1:D:1226:ARG:HB3	1.87	0.56
1:D:210:LYS:O	1:D:213:GLU:HG3	2.06	0.54
1:A:1134:TRP:CE2	1:A:1226:ARG:HD3	2.43	0.53
1:A:46:ASP:OD2	1:A:49[B]:SER:OG	2.26	0.53
1:A:1113:THR:HG21	1:A:1117:ILE:HD11	1.89	0.53
1:A:2119:HIS:H	6:A:3009:PEG:C3	2.20	0.52
1:D:2007:LEU:O	1:D:2008:ILE:HD13	2.09	0.52
1:D:2089:ILE:H	1:D:2089:ILE:HD12	1.75	0.51
1:D:1196[B]:ILE:HD11	1:D:2061:PRO:HA	1.93	0.51
1:A:2010:ARG:NH1	1:A:2021[B]:SER:OG	2.43	0.50
1:D:201:PHE:CE1	1:D:1102:MET:HG2	2.46	0.50
8:D:3006:1PE:H232	10:D:4183:HOH:O	2.11	0.50
2:A:3001:PGE:H5	10:A:4329:HOH:O	2.12	0.49
1:A:1122:SER:HB3	1:A:1128:PRO:HD3	1.95	0.48
1:A:1226:ARG:NH2	1:A:2003:LEU:HD12	2.29	0.47
1:A:1003:SER:HB2	1:A:1114:THR:HG22	1.97	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1047:LEU:HD13	1:A:1083[A]:LEU:HD11	1.98	0.46
1:D:2123:ILE:HG23	1:D:2194:ASN:ND2	2.31	0.46
1:D:1116:ARG:HH22	8:D:3008:1PE:H122	1.80	0.46
1:A:165[A]:ASP:OD2	1:A:167[A]:ARG:NH2	2.49	0.45
1:D:2018:PRO:HG2	1:D:2107:VAL:HG12	1.98	0.45
1:A:203:ARG:HG3	1:A:1179:HIS:O	2.17	0.45
1:A:1090:PRO:HD3	1:A:1096[A]:ILE:HD11	1.98	0.45
1:A:1124:SER:HA	1:A:1195:VAL:HG13	1.97	0.45
1:A:5:GLY:HA2	1:A:110:GLU:HG3	1.99	0.45
1:D:8:ILE:HD11	1:D:136:TRP:HZ3	1.81	0.44
1:D:2061:PRO:HD2	1:D:2080:THR:HG21	2.00	0.44
1:A:2037:ASP:HB3	1:A:2079:LYS:HG2	1.98	0.44
1:A:1200:ASP:O	1:A:1203:VAL:HG22	2.17	0.44
1:D:2003:LEU:HD22	1:D:2112:PRO:HA	2.00	0.43
2:D:3007:PGE:H22	7:D:3012:EDO:H22	2.01	0.43
1:A:165[A]:ASP:OD2	1:A:167[A]:ARG:NE	2.52	0.43
1:D:1012:SER:HB3	1:D:1018:PRO:HD3	2.02	0.42
1:A:208:THR:HB	1:D:2092[A]:MET:HG2	2.01	0.42
1:A:2072:ASN:HB3	1:A:2075:SER:HB2	2.00	0.42
1:D:1003:SER:HB2	1:D:1114:THR:HG22	2.01	0.42
1:A:185:GLU:OE1	1:D:68:ASN:N	2.48	0.42
1:D:2210:LYS:HG2	10:D:4014:HOH:O	2.19	0.42
1:A:79:LYS:HE3	1:D:77[A]:ASN:ND2	2.33	0.41
1:D:201:PHE:CZ	1:D:1102:MET:HG2	2.55	0.41
1:D:2060:LEU:HG	1:D:2176:GLY:CA	2.50	0.41
1:D:1024:THR:HG22	1:D:1113:THR:HB	2.03	0.41
1:D:2096:ASN:OD1	1:D:2097:ILE:N	2.51	0.41
1:A:10:ARG:HG3	10:A:4137:HOH:O	2.21	0.41
2:A:3008:PGE:H6	6:A:3009:PEG:H11	2.02	0.40
1:D:1155:GLY:HA3	1:D:2043:HIS:CE1	2.57	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	683/726 (94%)	669 (98%)	13 (2%)	1 (0%)	51	33
1	D	686/726 (94%)	669 (98%)	16 (2%)	1 (0%)	51	33
All	All	1369/1452 (94%)	1338 (98%)	29 (2%)	2 (0%)	51	33

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	22	ALA
1	A	96	ASN

5.3.2 Protein sidechains (i)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	589/618 (95%)	582 (99%)	7 (1%)	71	56
1	D	595/618 (96%)	590 (99%)	5 (1%)	81	72
All	All	1184/1236 (96%)	1172 (99%)	12 (1%)	76	63

All (12) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	67	GLN
1	A	86	ASN
1	A	1079	ASP
1	A	1113	THR
1	A	1181	ARG
1	A	2079	LYS
1	A	2086	ASN
1	D	213	GLU
1	D	1079	ASP
1	D	1113	THR
1	D	1181	ARG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	D	2079	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

5.3.3 RNA

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates

There are no monosaccharides in this entry.

5.6 Ligand geometry

Of 23 ligands modelled in this entry, 6 are monoatomic - leaving 17 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
2	PGE	D	3007	-	9,9,9	0.51	0	8,8,8	0.38	0
6	PEG	D	3010	-	6,6,6	0.50	0	5,5,5	0.23	0
7	EDO	D	3009	-	3,3,3	0.46	0	2,2,2	0.34	0
5	PG4	A	3005	-	12,12,12	0.53	0	11,11,11	0.28	0
7	EDO	D	3012	-	3,3,3	0.49	0	2,2,2	0.32	0
8	1PE	D	3006	-	15,15,15	0.54	0	14,14,14	0.36	0
6	PEG	A	3007	-	6,6,6	0.48	0	5,5,5	0.26	0
2	PGE	D	3005	-	9,9,9	0.51	0	8,8,8	0.22	0
7	EDO	D	3011	-	3,3,3	0.48	0	2,2,2	0.36	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
2	PGE	A	3001	-	9,9,9	0.74	0	8,8,8	0.92	1 (12%)
2	PGE	A	3006	-	9,9,9	0.51	0	8,8,8	0.28	0
8	1PE	D	3008	-	15,15,15	0.54	0	14,14,14	0.33	0
5	PG4	D	3004	-	12,12,12	0.52	0	11,11,11	0.33	0
9	PO4	D	3013	-	4,4,4	1.06	0	6,6,6	0.56	0
7	EDO	A	3010	-	3,3,3	0.47	0	2,2,2	0.36	0
6	PEG	A	3009	-	6,6,6	0.52	0	5,5,5	0.60	0
2	PGE	A	3008	-	9,9,9	0.48	0	8,8,8	0.29	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	PGE	D	3007	-	-	4/7/7/7	-
6	PEG	D	3010	-	-	2/4/4/4	-
7	EDO	D	3009	-	-	1/1/1/1	-
5	PG4	A	3005	-	-	2/10/10/10	-
7	EDO	D	3012	-	-	0/1/1/1	-
8	1PE	D	3006	-	-	9/13/13/13	-
6	PEG	A	3007	-	-	3/4/4/4	-
2	PGE	D	3005	-	-	3/7/7/7	-
7	EDO	D	3011	-	-	0/1/1/1	-
2	PGE	A	3001	-	-	5/7/7/7	-
2	PGE	A	3006	-	-	4/7/7/7	-
8	1PE	D	3008	-	-	5/13/13/13	-
5	PG4	D	3004	-	-	5/10/10/10	-
7	EDO	A	3010	-	-	1/1/1/1	-
6	PEG	A	3009	-	-	2/4/4/4	-
2	PGE	A	3008	-	-	0/7/7/7	-

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	3001	PGE	O3-C5-C6	2.15	119.53	110.07

There are no chirality outliers.

All (46) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	D	3007	PGE	C1-C2-O2-C3
6	A	3009	PEG	O2-C3-C4-O4
2	D	3005	PGE	O2-C3-C4-O3
8	D	3008	1PE	OH6-C15-C25-OH5
5	D	3004	PG4	O2-C3-C4-O3
2	A	3001	PGE	O2-C3-C4-O3
8	D	3008	1PE	OH5-C14-C24-OH4
8	D	3006	1PE	OH4-C13-C23-OH3
6	D	3010	PEG	O2-C3-C4-O4
8	D	3006	1PE	OH7-C16-C26-OH6
2	A	3001	PGE	O1-C1-C2-O2
5	D	3004	PG4	O1-C1-C2-O2
2	D	3005	PGE	O1-C1-C2-O2
2	D	3007	PGE	O3-C5-C6-O4
8	D	3006	1PE	C12-C22-OH3-C23
5	D	3004	PG4	C3-C4-O3-C5
7	A	3010	EDO	O1-C1-C2-O2
7	D	3009	EDO	O1-C1-C2-O2
5	D	3004	PG4	O3-C5-C6-O4
6	A	3007	PEG	O2-C3-C4-O4
8	D	3006	1PE	OH2-C12-C22-OH3
8	D	3006	1PE	OH5-C14-C24-OH4
2	A	3006	PGE	O2-C3-C4-O3
2	A	3006	PGE	C3-C4-O3-C5
5	D	3004	PG4	C4-C3-O2-C2
8	D	3006	1PE	C25-C15-OH6-C26
8	D	3008	1PE	C23-C13-OH4-C24
8	D	3008	1PE	OH7-C16-C26-OH6
6	A	3009	PEG	C4-C3-O2-C2
5	A	3005	PG4	C6-C5-O3-C4
2	D	3005	PGE	C4-C3-O2-C2
2	A	3001	PGE	C3-C4-O3-C5
2	A	3001	PGE	O3-C5-C6-O4
6	A	3007	PEG	O1-C1-C2-O2
2	A	3006	PGE	C1-C2-O2-C3
8	D	3006	1PE	C24-C14-OH5-C25
6	D	3010	PEG	C4-C3-O2-C2
6	A	3007	PEG	C4-C3-O2-C2
8	D	3006	1PE	C23-C13-OH4-C24
8	D	3006	1PE	C15-C25-OH5-C14
2	A	3001	PGE	C1-C2-O2-C3
2	D	3007	PGE	C3-C4-O3-C5

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
2	A	3006	PGE	C6-C5-O3-C4
8	D	3008	1PE	OH2-C12-C22-OH3
5	A	3005	PG4	C3-C4-O3-C5
2	D	3007	PGE	O2-C3-C4-O3

There are no ring outliers.

7 monomers are involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	D	3007	PGE	1	0
7	D	3012	EDO	1	0
8	D	3006	1PE	1	0
2	A	3001	PGE	1	0
8	D	3008	1PE	1	0
6	A	3009	PEG	4	0
2	A	3008	PGE	1	0

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95^{th} percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	A	674/726 (92%)	-0.29	15 (2%)	62	69	9, 19, 38, 64	0
1	D	676/726 (93%)	-0.03	26 (3%)	40	47	10, 21, 40, 64	0
All	All	1350/1452 (92%)	-0.16	41 (3%)	50	56	9, 20, 39, 64	0

All (41) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	22	ALA	7.7
1	D	23	GLY	6.4
1	A	2022	ALA	5.2
1	D	2002	TYR	4.4
1	D	3	LEU	4.2
1	A	2003	LEU	4.1
1	D	1091	MET	4.1
1	D	197	SER	3.9
1	A	2004	THR	3.7
1	D	227	ASN	3.7
1	D	21	SER	3.7
1	A	2197	SER	3.5
1	A	8	ILE	3.4
1	D	200	PRO	3.3
1	D	2097	ILE	3.3
1	D	4	THR	3.1
1	D	215	GLN	3.0
1	D	1227	ARG	3.0
1	D	20	CYS	3.0
1	D	25	THR	3.0
1	A	4	THR	2.9
1	A	227	ASN	2.9
1	D	111	ALA	2.8
1	D	2227	ASN	2.7

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	D	2086	ASN	2.6
1	A	2199	GLN	2.5
1	A	23	GLY	2.5
1	A	2002	TYR	2.4
1	A	213	GLU	2.4
1	D	130	ASN	2.3
1	A	91	MET	2.3
1	D	8	ILE	2.2
1	D	2130	ASN	2.2
1	D	2023	GLY	2.2
1	D	113	ALA	2.2
1	D	2003	LEU	2.2
1	A	197	SER	2.1
1	D	19	ALA	2.1
1	A	1091	MET	2.1
1	D	112	PRO	2.1
1	A	68	ASN	2.0

6.2 Non-standard residues in protein, DNA, RNA chains (i)

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	PGE	D	3005	10/10	0.58	0.20	56,61,65,67	0
2	PGE	A	3006	10/10	0.70	0.21	54,59,66,70	0
7	EDO	D	3012	4/4	0.75	0.20	45,47,50,53	0
5	PG4	A	3005	13/13	0.76	0.20	43,49,55,56	0
2	PGE	D	3007	10/10	0.76	0.17	43,51,54,54	0
6	PEG	A	3007	7/7	0.77	0.17	46,49,55,61	0

Continued on next page...

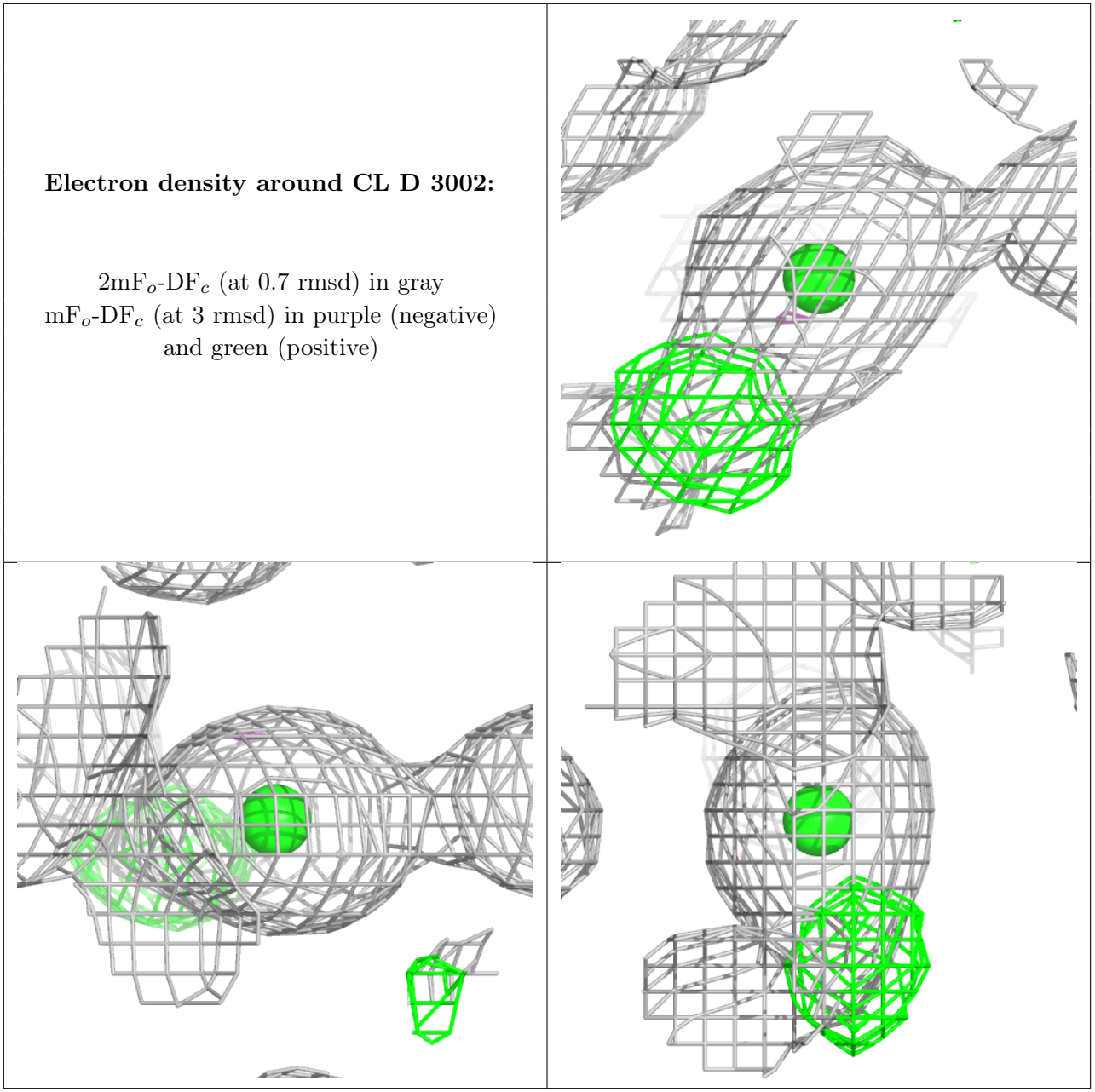
Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
6	PEG	D	3010	7/7	0.83	0.19	51,52,56,60	0
5	PG4	D	3004	13/13	0.84	0.20	34,37,43,44	0
8	1PE	D	3006	16/16	0.84	0.26	38,46,59,59	0
2	PGE	A	3001	10/10	0.85	0.12	37,44,48,51	0
7	EDO	A	3010	4/4	0.86	0.12	42,48,51,53	0
7	EDO	D	3011	4/4	0.86	0.10	53,54,54,54	0
8	1PE	D	3008	16/16	0.86	0.15	35,46,57,59	0
6	PEG	A	3009	7/7	0.87	0.27	24,28,32,45	0
7	EDO	D	3009	4/4	0.88	0.15	41,43,46,47	0
2	PGE	A	3008	10/10	0.95	0.13	31,32,41,51	0
3	CL	D	3002	1/1	0.98	0.05	28,28,28,28	0
9	PO4	D	3013	5/5	0.98	0.06	27,29,32,35	5
3	CL	A	3003	1/1	0.99	0.05	19,19,19,19	0
4	MG	A	3004	1/1	0.99	0.05	15,15,15,15	0
4	MG	D	3003	1/1	0.99	0.03	14,14,14,14	0
3	CL	D	3001	1/1	1.00	0.06	12,12,12,12	0
3	CL	A	3002	1/1	1.00	0.05	13,13,13,13	0

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

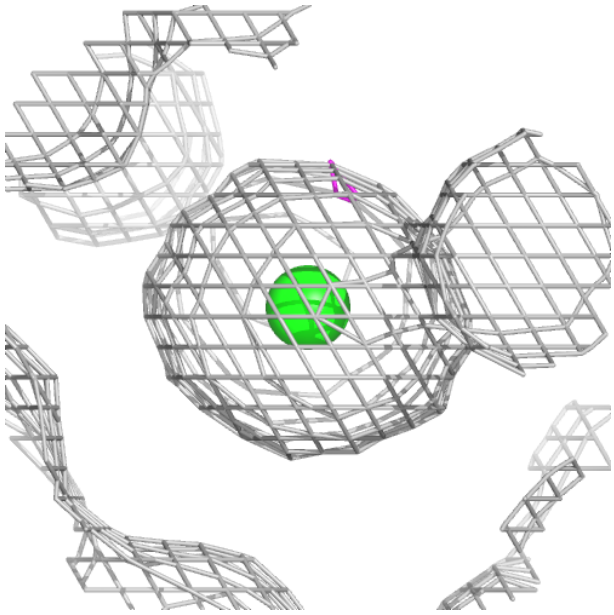
Electron density around CL D 3002:

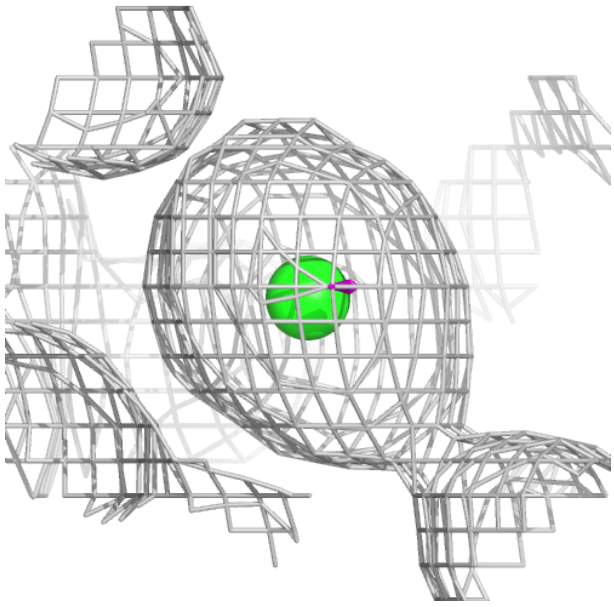
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

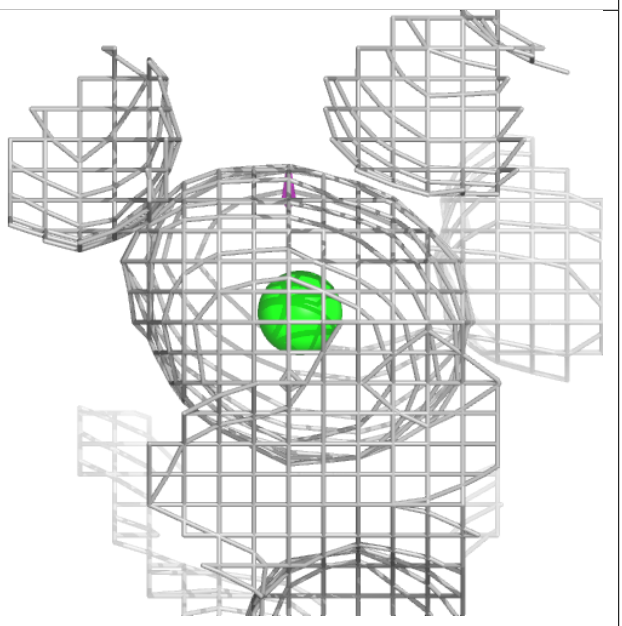


Electron density around CL A 3003:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

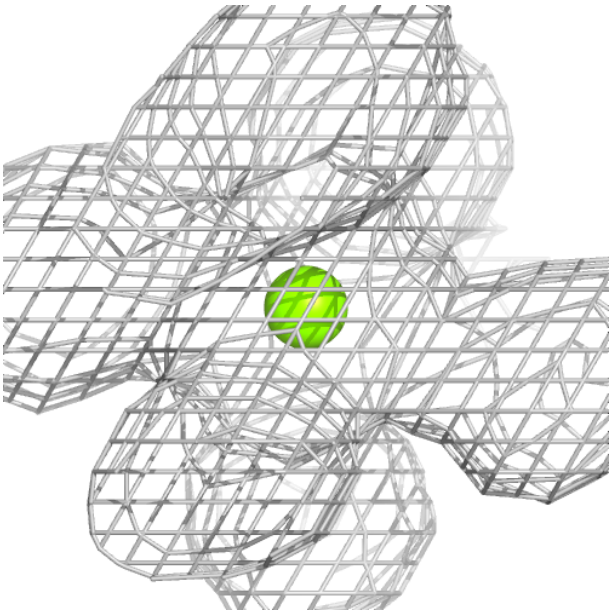


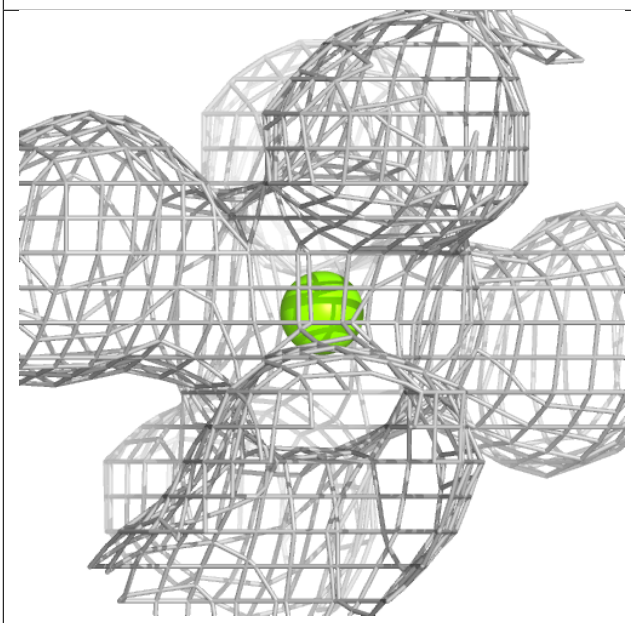


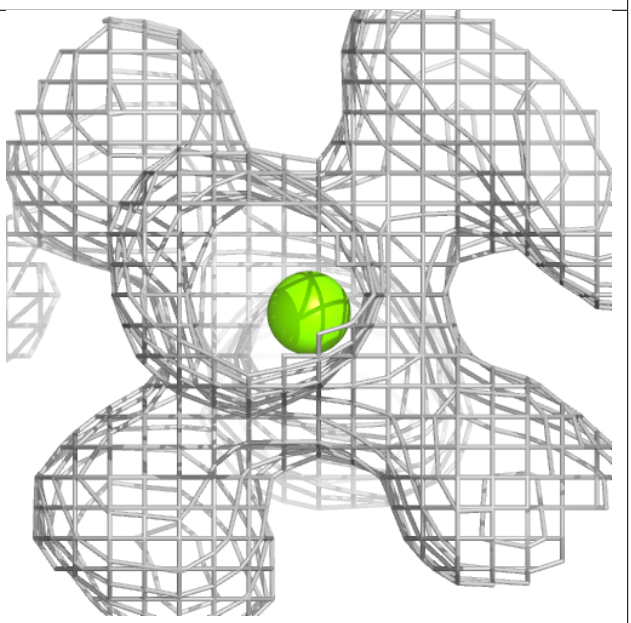


Electron density around MG A 3004:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

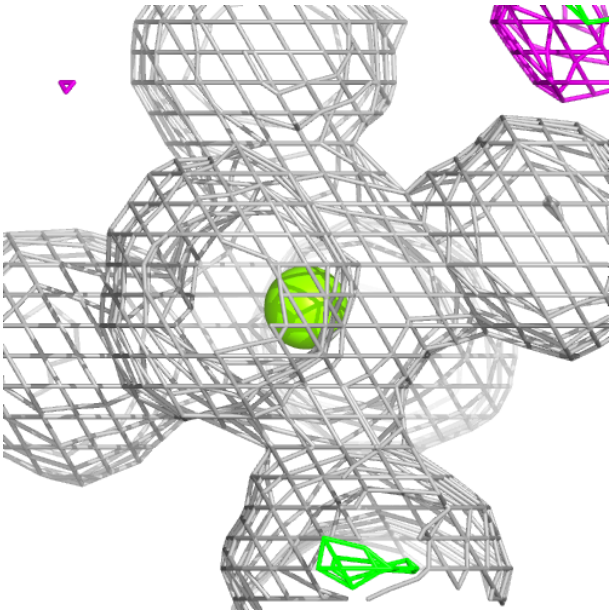


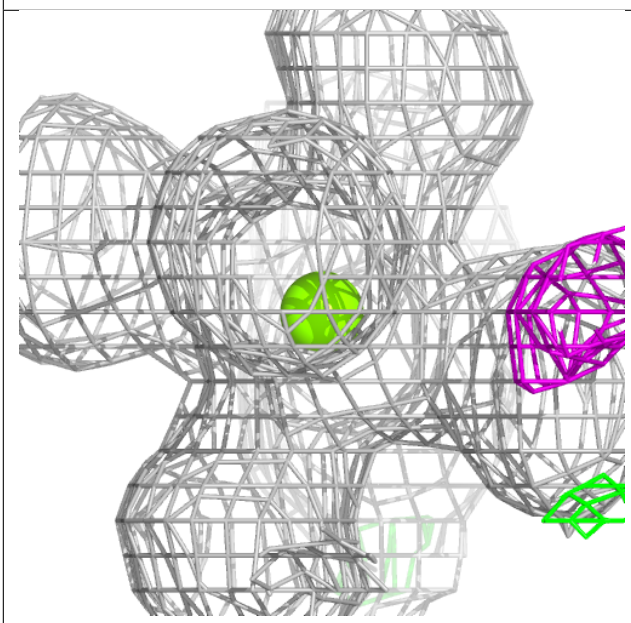


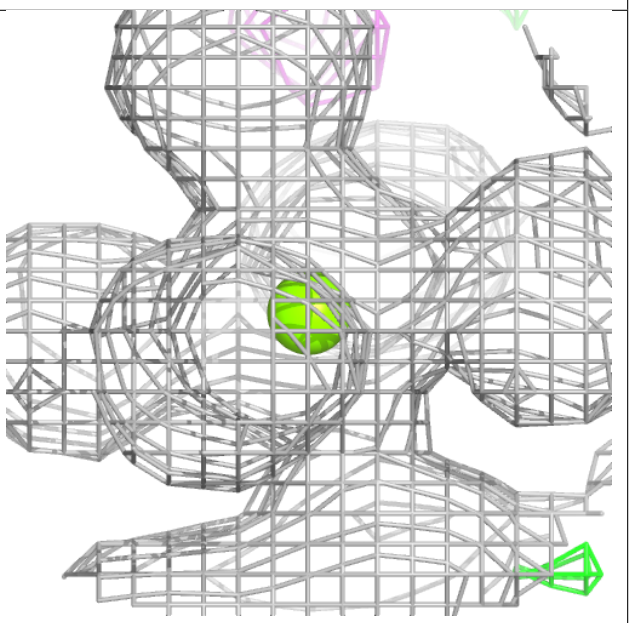


Electron density around MG D 3003:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

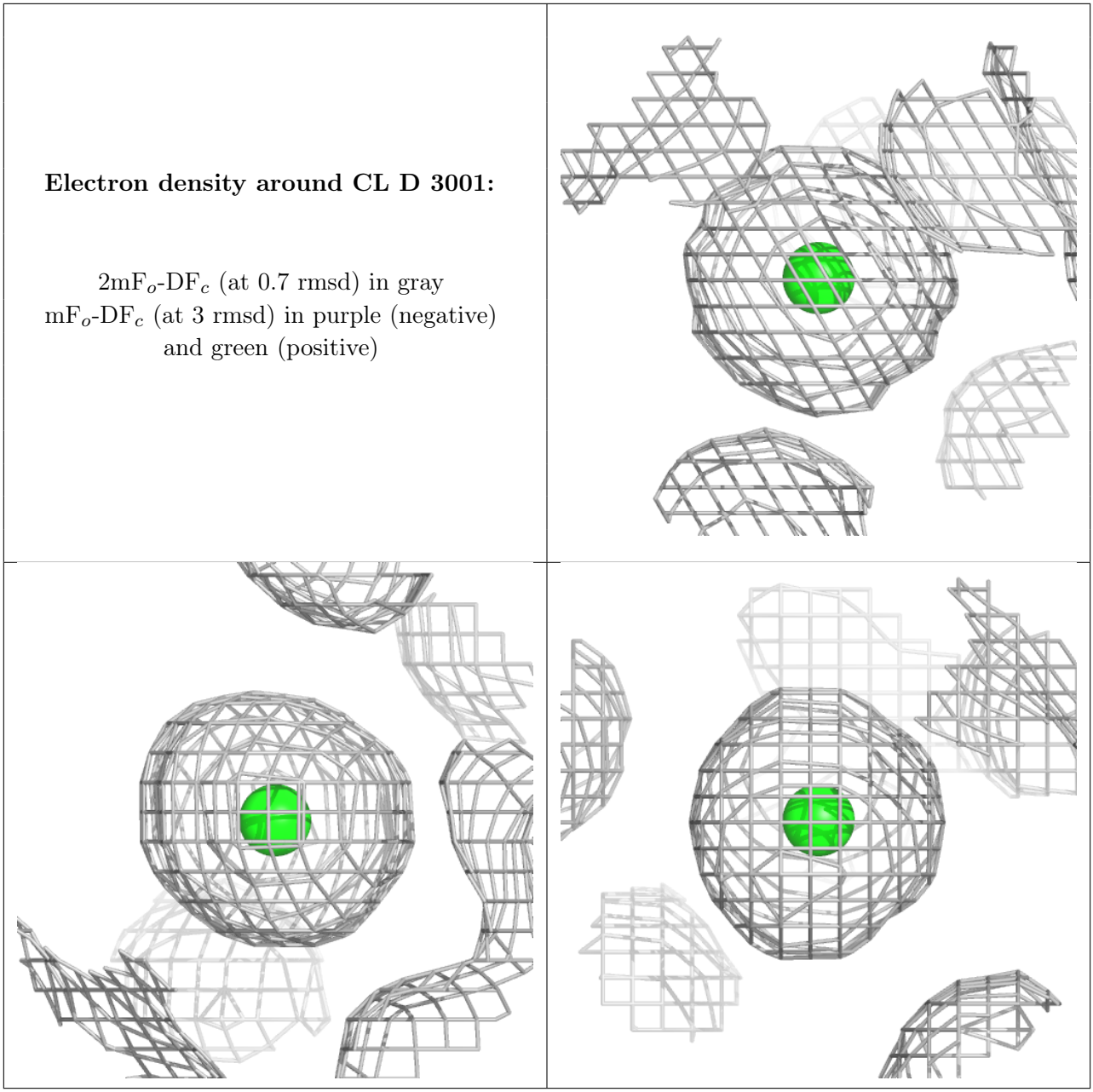






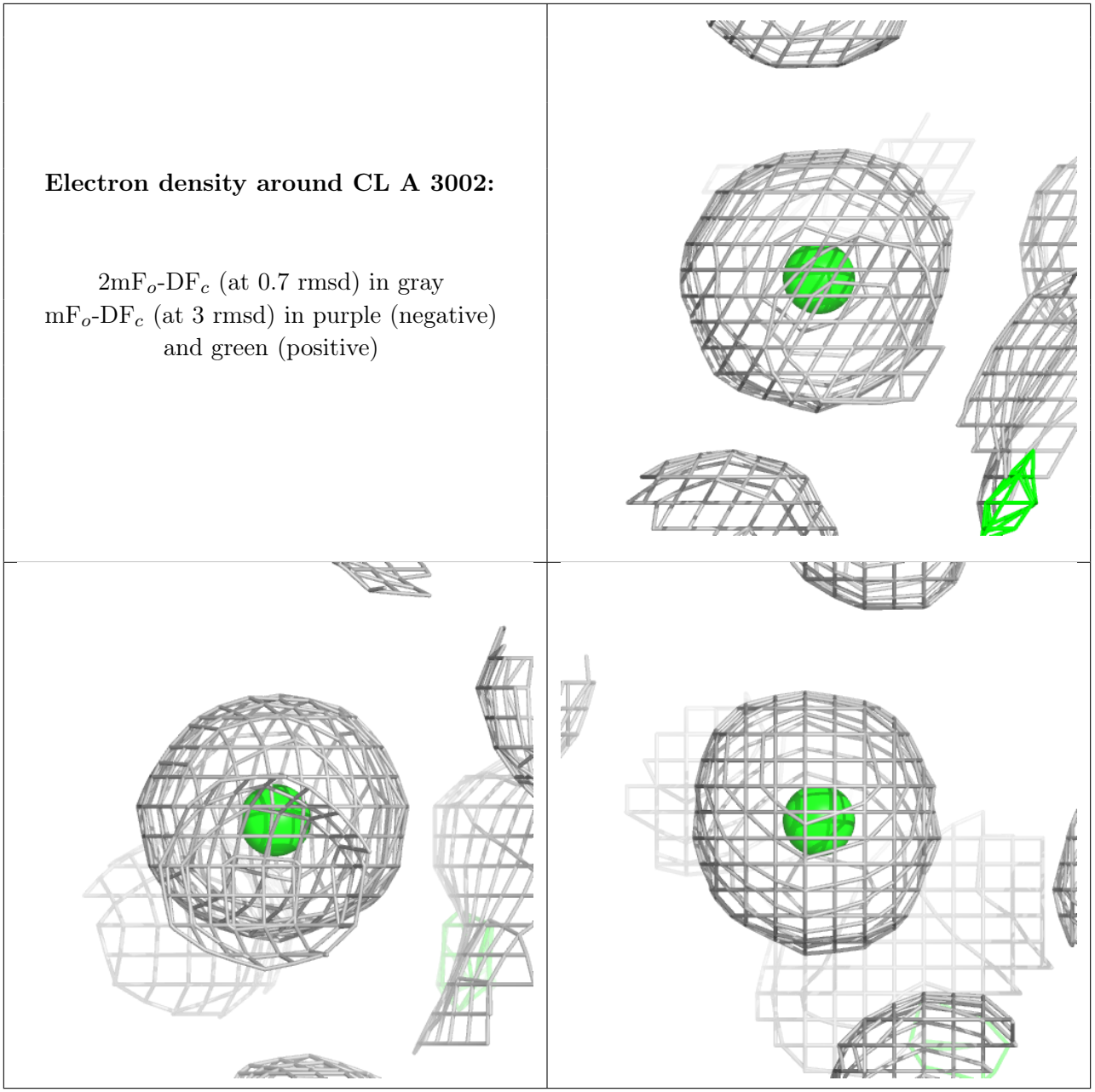
Electron density around CL D 3001:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)



Electron density around CL A 3002:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)



6.5 Other polymers (i)

There are no such residues in this entry.